Input Files for Computer Simulation of Water Radiolysis

Bjergbakke, Erling; Sehested, Knud; Lang Rasmussen, Ole; Christensen, H.

Publication date:
1984

Document Version
Publisher's PDF, also known as Version of record

RISØ-M-2430

RISØ-M-2430

RISØ

Input Files for Computer Simulation of Water Radiolysis

E. Bjergbakke, K. Sehested, O. Lang Rasmussen,
H. Christensen

Risø National Laboratory, DK-4000 Roskilde, Denmark
April 1984

RISØ-M-2430

INPUT FILES FOR COMPUTER SIMULATION OF WATER RADIOLYSIS

E. Bjergbakke and K. Sehested, Accelerator Department
O. Lang Rasmussen, Computer Installation
H. Christensen, Studsvik Energiteknik AB, Sweden

Abstract. This report contains radiation chemistry input files for CHEMSIMUL, a program package for numerical simulation of chemical reaction systems.

INIS-descriptors: CARBONATES; CHEMICAL REACTION KINETICS; CHLORIDES; COMPUTERIZED SIMULATION; G VALUE; IRON COMPOUNDS; RADIOLYSIS; WATER

UDC 681.3.06 : 546.212 : 541.15

April 1984
Risø National Laboratory, DK 4000 Roskilde, Denmark

ISBN 87-550-1001-6
ISSN 0418-6435

Risø Repro 1984

CONTENTS

1. INTRODUCTION

Over the years we have constructed a series of input files for computer-simulation (1) of water radiolysis experiments. These files have proved adequate for simulation of our experimental results. The files are continously objects for revisions as reactions and rate constants become better known.

The reaction equations are numbered in succession in order to facilitate addition of files. The rate constants are written after each equation separated with ";". The unit for the rate constant derives from the left-hand side of the equation. If there is only one reactant the unit is s^{-1}, if there are two the unit is $dm^3mol^{-1}s^{-1}$. If the two reactants are identical the rate constant is given as 1k.

In order to preserve the mass, the water concentration is included in the computations and reactions with water are second-order reactions.

Note that E[-] symbolize one electron plus one water molecule. Where no reference is given the rate constants are chosen from the NBS-tables (2,3,4,5,6).

The G-value files are constructed with a complete preservation of mass and charge:

Hydrogen balance

$$-G(H2O)=0.5*G(OH)+0.5*G(H)+G(H2)+G(H2O2)+0.5*G(H[+])+0.5*G(OH[-])+G(E[-]$$

Oxygen balance

$$-G(H2O)=G(OH)+2G(H2O2)+G(OH[-])+G(E[-])$$

Charge balance

$$G(H[+])=G(E[-])+G(OH[-])$$

2. WATER REACTIONS

FILENAME=EB/WATER

This file contains reactions for simulation of radiolysis of acid, neutral and alkaline water.

	References and notes
RE1:OH+OH=H2O2;6E9	
RE2:OH+E[-]=OH[-]+H2O;2.5E10	
RE3:OH+H=H2O;2.5E10	
RE4:OH+O[-]=HO2[-];1.8E10	
RE5:OH+HO2=H2O3;7.9E9	
RE6:OH+O2[-]=OH[-]+O2;E10	
RE7:OH+O3[-]=O3+OH[-];2.5E9	(7)
RE8:OH+O3[-]=HO2+O2[-];6E9	(7)
RE9:OH+H2O2=H2O+O2[-]+H[+];2.7E7	
RE10:OH+HO2[-]=H2O+O2[-];7.5E9	(8)
RE11:OH+OH[-]=O[-]+H2O;1.4E10	
RE12:OH+H2=H2O+H;4E7	
RE13:OH+O3=O2[-]+O2+H[+];E8	(9)
RE19:E[-]+E[-]=2*OH[-]+H2;3E9	
RE20:E[-]+H=OH[-]+H2;2E10	
RE21:E[-]+O[-]=2*OH[-];1.5E10	
RE22:E[-]+O2[-]=HO2[-]+OH[-];1.2E10	
RE23:E[-]+H2O2=OH+OH[-]+H2O;1.6E10	
RE24:E[-]+HO2[-]=O[-]+OH[-]+H2O;3.5E9	
RE25:E[-]+H[+]=H+H2O;2.2E10	
RE26:E[-]+O2=O2[-]+H2O;2E10	
RE27:E[-]+O3=O3[-]+H2O;3.6E10	(10)
RE28:E[-]+N2O=O[-]+N2+H2O;9E9	
RE31:H+H=H2;E10	
RE32:H+HO2=H2O2;2E10	
RE33:H+O2[-]=HO2[-];2E10	
RE34:H+H2O2=OH+H2O;6E7	
RE35:H+OH[-]=E[-];1.5E7	
RE36:H+O2=O2[-]+H[+];2E10	
RE37:H+O3=OH+O2;3.6E10	(10)

RE38:H+O[-]=OH[-];2E10	
RE43:O[-]+O[-]=O2[--];9E8	
RE44:O[-]+O2[-]=O3[--];3.5E8	(11)
RE45:O[-]+O3[-]=2*O2[-];3.5E8	(11)
RE46:O[-]+H2O2=O2[-]+H2O;5E8	(8)
RE47:O[-]+HO2[-]=OH[-]+O2[-];3.5E8	(8)
RE48:O[-]+H2O=OH+OH[-];2E6	
RE49:O[-]+O2=O3[-];3.0E9	
RE50:O[-]+H2=OH[-]+H;2E8	(12)
RE56:HO2=O2[-]+H[+];8E5	
RE57:HO2+HO2=O2+H2O2;7.5E5	
RE58:HO2+O2[-]=O2+HO2[-];E8	
RE61:O2[-]+H[+]=HO2;5E10	
RE62:O2[-]+O3=O3[-]+O2;1.5E9	(10)
RE64:H2O3=O2+H2O;2.1	(13)
RE65:O3[-]=O[-]+O2;3.3E3	(14)
RE66:O3[-]+H[+]=OH+O2;9E10	(7)
RE68:H2O2+OH[-]=HO2[-]+H2O;5E8	
RE69:HO2[-]+H2O=H2O2+OH[-];5.735E4	
RE70:HO2[-]+O3=O3[-]+O2[-]+H[+];3E6	(15)
RE73:H2O=H[+]+OH[-];2.599E-5	
RE74:H2O+O2[--]=HO2[-]+OH[-];E8	(a)
RE75:H2O+O3[--]=O2+2*OH[-];E8	(a)
RE76:H[+]+OH[-]=H2O;1.43E11	

Notes:

(a) Balance reactions of no significance for the kinetics.

3. CARBONATE REACTIONS

FILENAME=EB/CARBONATE

This file contains reactions that are used for simulation of radiolysis of carbonate in aqueous solution when combined with EB/WATER.

	References and notes
RE80:OH+CO3[--]=CO3[-]+OH[-];4E8	
RE81:OH+HCO3[-]=CO3[-]+H2O;1.5E7	
RE82:O2[-]+CO3[-]=CO3[--]+O2;3.2E8	(a)
RE83:H2O2+CO3[-]=CO3[--]+O2[-]+2*H[+];4.3E5	(a)
RE84:HO2[-]+CO3[-]=CO3[--]+O2[-]+H[+];3E7	(a)
RE85:O3[-]+CO3[-]=CO3[--]+O3;6E7	(16)
RE86:H[+]+HCO3[-]=CO2+H2O;E10	(b)
RE87:OH[-]+HCO3[-]=CO3[--]+H2O;E9	(c)
RE88:H2O+CO2=HCO3[-]+H[+];70	(b)
RE89:H2O+CO3[--]=HCO3[-]+OH[-];3.6E3	(c)
RE90:H2O+CO4[--]=HO2[-]+OH[-]+CO2;0.2	(a)
RE91:CO3[-]+CO3[-]=CO4[--]+CO2;7E6	

Notes:

(a) K.Sehested, to be published.

(b) pK(CO2/HCO3[-]) = 6.4.

(c) pK(HCO3[-]/CO3[--]) = 10.3.

4. FERROUS REACTIONS

FILENAME=EB/FE

This file contains reactions that are used for simulation of radiolysis of ferrous/ferric in acid aqueous solution when combined with EB/WATER.

	References and notes
RE105:FE[++]+OH=FE[+++]+OH[-];3.4E8	
RE106:FE[++]+E[-]=FE[+++]+OH[-]+H[-];1.2E8	
RE107:FE[+++]+E[-]=FE[++]+H2O;2E10	
RE108:FE[++]+H=FE[+++]+H[-];1.3E7	
RE109:FE[+++]+H=FE[++]+H[+];1E8	
RE110:FE[++]+HO2=FE[+++]+HO2[-];1.6E6	
RE111:FE[++]+O2[-]=FE[+++]+O2[--];2E8	(a)
RE112:FE[+++]+O2[-]=FE[++]+O2;5E8	(a)
RE113:FE[++]+H2O2=FE[+++]+OH+OH[-];62	(17)
RE114:FE[++]+H2O3=FE[+++]+HO2+OH[-];6E4	(18)
RE115:H[-]+H2O=H2+OH[-];E6	(b)
RE116:O2[--]+H2O=HO2[-]+OH[-];E6	(b)

Notes:

(a) Calculated from refs. (18) and (19).

(b) Balance reactions of no significance for the kinetics.

5. CHLORIDE REACTIONS

FILENAME=EB/CHLORIDE

This file contains reactions that are used for simulation of radiolysis of chloride in acid and neutral aqueous solution when combined with EB/WATER.

	References and notes
RE125:OH+CL[-]=CLOH[-];4.3E9	
RE126:OH+HCLO=CLO+H2O;9E9	
RE127:OH+HCLO2=CLO2+H2O;6.3E9	
RE128:E[-]+CL=CL[-]+H2O;E10	
RE129:E[-]+CL2[-]=2*CL[-]+H2O;E10	
RE130:E[-]+CLOH[-]=CL[-]+OH[-]+H2O;E10	(a)
RE131:E[-]+HCLO=CLOH[-]+H2O;5.3E10	
RE132:E[-]+CL2=CL2[-]+H2O;E10	(a)
RE133:E[-]+CL3[-]=CL2[-]+CL[-]+H2O;E10	(a)
RE134:E[-]+HCLO2=CLO+OH[-]+H2O:4.5E10	
RE135:E[-]+HCLO3=CLO2+OH[-]+H2O;4E6	
RE136:H+CL=CL[-]+H[+];E10	(a)
RE137:H+CL2[-]=2*CL[-]+H[+];8E9	(20)
RE138:H+CLOH[-]=CL[-]+H2O;E10	
RE139:H+CL2=CL2[-]+H[+];7E9	(20)
RE140:H+HCLO=CLOH[-]+H[+];E10	
RE141:H+CL3[-]=CL2[-]+CL[-]+H[+];E10	
RE142:HO2+CL2[-]=2*CL[-]+O2+H[+];4E9	
RE143:HO2+CL2=CL2[-]+O2+H[+];E9	(21)
RE144:HO2+CL3[-]=CL2[-]+CL[-]+O2+H[+];E9	
RE145:O2[-]+CL2[-]=2*CL[-]+O2;1.2E10	(20)
RE146:O2[-]+HCLO=CLOH[-]+O2;7.5E6	(22)
RE147:H2O2+CL2[-]=2*CL[-]+O2[-]+2*H[+];1.4E5	(23)
RE148:H2O2+CL2=HO2+CL2[-]+H[+];1.9E2	(24)
RE149:H2O2+HCLO=CL[-]+O2+H2O+H[+];1.7E5	(25)
RE150:OH[-]+CL2[-]=CLOH[-]+CL[-];7.3E6	(23)
RE151:OH[-]+CL2=HCLO+CL[-];3.88E11	(b)
RE152:H[+]+CLOH[-]=CL+H2O;2.1E10	(26)
RE153:H2O+CL2O2=HCLO+HCLO2;2E2	(a)
RE154:H2O+CL2O2=O2+HCLO+CL[-]+H[+];E2	(a)

RE155:H2O+CL2O=2*HCLO;E2 (a)

RE156:H2O+CL2O4=HCLO2+HCLO3;E2 (a)

RE157:H2O+CL2O4=2*O2+HCLO+CL[-]+H[+];E2 (a)

RE158:CL[-]+CL=CL2[-];2.1E10 (26)

RE159:CL[-]+CLOH[-]=CL2[-]+OH[-];9E4 (27)

RE160:CL[-]+HCLO=CL2+OH[-];10 (b)

RE161:CL[-]+CL2=CL3[-];1E4 (c)

RE162:CLOH[-]=OH+CL[-];6.1E9 (26)

RE163:CL2[-]=CL+CL[-];1.1E5 (26)

RE164:CL2[-]+CL2[-]=CL3[-]+CL[-];7E9

RE165:CL3[-]=CL2+CL[-];5E4 (c)

RE166:CLO+CLO=CL2O2;1.5E10

RE167:CLO2+CLO2=CL2O4;E2 (a)

RE168:CL2O2+HCLO2=HCLO3+CL2O;E2 (a)

Notes:

(a) Reaction not known, arbitrary rate constant.

(b) Based on eq.constant for Cl2+H2O=HClO+Cl[-]+H[+];K=3.88E-4, ref. (28).

(c) Based on eq.constant for Cl2+Cl[-]=Cl3[-];K=0.18, ref. (28).

6. Fe-Cl REACTIONS

FILENAME=EB/FECL

This file contains reactions that are used for simulation of radiolysis of chloride + ferrous/ferric in aqueous solution when combined with EB/WATER, EB/FE, and EB/CHLORIDE.

	References and notes
RE170:CL+FE[++]=FE[+++]+CL[-];1.05E10	(29)
RE171:CLOH[-]+FE[++]=FE[+++]+CL[-]+OH[-];E8	
RE172:CL2[-]+FE[++]=FE[+++]+2*CL[-];1E7	
RE173:CL2+FE[++]=FE[+++]+CL2[-];80	(30)
RE174:HCLO+FE[++]=FE[+++]+CLOH[-];3.6E3	(30)
RE175:CL3[-]+FE[++]=FE[+++]+CL2[-]+CL[-];2E5	(a)

Notes:

(a) Estimated from ref. (31).

7. OZONE REACTIONS

FILENAME = EB/OZONE

This file contains reactions that are used for simulation of radiolysis of ozone in neutral and alkaline aqueous solution when combined with EB/WATER.

	References and notes
RE180:OH+O3=O2[-]+O2+H[+];1.1E8	(9)
RE181:E[-]+O3=O3[-]+H2O;3.6E10	(10)
RE182:H+O3=OH+O2;3.65E10	(10)
RE183:O[-]+O3=O2[-]+O2;E9	(a)
RE184:O2[-]+O3=O3[-]+O2;1.52E9	(10)
RE185:HO2[-]+O3=O3[-]+O2[-]+H[+];3E6	(32)

Notes:

(a) Estimated rate constant.

8. HIGH TEMPERATURE WATER REACTIONS

FILENAME=EB/H2OTEMP

This file is used for simulation of radiolysis of water at high temperature (temperature constant or a function of time). After each reaction equation the activation energy E_a (kcal*mol^{-1}) and the frequency factor A are separated by a comma in writing. Where no reference is mentioned E_a is taken from Jenks estimated values (33,34). A is calculated from the rate constant at room temperature. The rate constants at T degree Kelvin is calculated from the Arrhenius equation:

$$k = A*e^{-503.3*E_a/T}$$

References and notes

RE1:OH+OH=H2O2;3,6.57E11
RE2:OH+E[-]=OH[-]+H2O;3,3.28E12
RE3:OH+H=H2O;3,4.1E12
RE4:OH+HO2=O2+H2O;3,1.3E12
RE5:OH+O2[-]=O2+OH[-];3,1.64E12
RE6:OH+H2O2=H2O+HO2;3.4,4.74E10 (8)
RE7:OH+H2=H+H2O;4.6,8.44E10 (35)
RE8:E[-]+E[-]=2*OH[-]+H2;5.3,4.1E13
RE9:E[-]+H=OH[-]+H2;3,3.28E12
RE10:E[-]+HO2=H2O2+OH[-];3,3.28E12
RE11:E[-]+O2[-]=HO2[-]+OH[-];4.5,2.74E13
RE12:E[-]+H2O2=OH+OH[-]+H2O;3,2.63E12
RE13:E[-]+H[+]=H+H2O;3,3.61E12
RE14:E[-]+H2O=H+OH[-]+H2O;3,3.28E3
RE15:E[-]+O2=O2[-]+H2O;3,3.28E12
RE16:H+H=H2;3,1.64E12
RE17:H+HO2=H2O2;3,3.28E12
RE18:H+O2[-]=HO2[-];3,3.28E12
RE19:H+H2O2=OH+H2O;4.5,1.26E11
RE20:H+OH[-]=E[-];3,3.28E9
RE21:H+O2=HO2;3,3.28E12
RE22:HO2+O2[-]=O2+HO2[-];4.5,1.79E11
RE23:HO2=O2[-]+H[+];3,1.31E8

RE24:O2[-]+H[+]=HO2;3,8.21E12

RE25:H2O2+OH[-]=HO2[-]+H2O;4.5,1.05E12

RE26:HO2[-]+H2O=H2O2+OH[-];3,9.42E6

RE27:H2O2=H2O+O;17,3.78E7

RE28:O+O=O2;3,1.64E12

RE29:H[+]+OH[-]=H2O;3,2.35E13

RE30:H2O=H[+]+OH[-];3,4.27E-3

9. G-VALUES

FILENAME=EB/GAMMA

This file contains G-values for low-LET electron and gamma irradiation of neutral water, ref. (36).

G(OH)=2.67
G(E[-])=2.66
G(H)=0.55
G(H2)=0.45
G(H2O2)=0.72
G(H[+])=2.76
G(OH[-])=0.1
G(H2O)=-6.87

FILENAME=EB/GAMMAPH046

This file contains G-values for low-LET electron and gamma irradiation of water pH=0.46, ref. (36).

G(OH)=2.89
G(H)=3.62
G(H2)=0.395
G(H2O2)=0.76
G(H[+])=0.1
G(OH[-])=0.1
G(H2O)=-4.51

FILENAME=EB/GAMMAPH1

This file contains G-values for low-LET electron and gamma irradiation of water pH=1, ref. (36).

G(OH)=2.83
G(H)=3.55
G(H2)=0.40
G(H2O2)=0.76
G(H[+])=0.1
G(OH[-])=0.1
G(H2O)=-4.45

FILENAME=EB/GAMMAPH2

This file contains G-values for low-LET electron and gamma irradiation of water pH=2, ref. (36).

G(OH)=2.74
G(E[-])=2.80
G(H)=0.55
G(H2)=0.425
G(H2O2)=0.73
G(H[+])=2.90
G(OH[-])=0.1
G(H2O)=-7.10

FILENAME=EB/GAMMAPH13

This file contains G-values for low-LET electron and gamma irradiation of water pH=13, refs. (36,11).

G(OH)=3.0
G(E[-])=2.8
G(H)=0.55
G(H2)=0.425
G(HO2[-])=0.6
G(H[+])=3.90
G(OH[-])=0.5
G(H2O)=-7.50

FILENAME=EB/GAMMAPH14

This file contains G-values for low-LET electron and gamma irradiation of water pH=14, refs. (36,11).

G(OH)=3.3
G(E[-])=2.8
G(H)=0.55
G(H2)=0.425
G(HO2[-])=0.45
G(H[+])=3.75
G(OH[-])=0.5
G(H2O)=-7.50

FILENAME=EB/N2OPH13

This file contains G-values for low-LET electron and gamma irradiation of water pH=13, equilibrated with 4 MPa N_2O, refs. (36,11).

G(E[-])=3.7
G(H)=0.55
G(OH)=3.4
G(HO2[-])=0.6
G(H2)=0.175
G(H[+])=4.8
G(OH[-]=0.5
G(H2O)=-8.80

FILENAME=EB/ALFA

This file contains G-values for alfa irradiated neutral water. Based on refs. (37,38,39,40) and best fit to experiments, ref. (41).

G(OH)=.24
G(E[-])=.06
G(H)=0.21
G(H2)=1.3
G(H2O2)=0.985
G(HO2)=0.22
G(H[+])=0.06
G(H2O)=-2.71

FILENAME=EB/NEUTRON

This file contains G-values for neutron irradiated neutral water, ref. (37).

G(OH)=0.46
G(E[-])=0.37
G(H)=0.36
G(H2)=1.12
G(H2O2)=1.00
G(HO2)=0.17
G(H[+])=0.37
G(H2O)=-3.17

REFERENCES

(1) O.Lang Rasmussen and E. Bjergbakke, Risø-R-395 (1984).

(2) M. Anbar, M. Bambenek and A.B. Ross, NSRDS-NBS 43 (1973) and suppl. (1975).

(3) L.M. Dorfman and G.E. Adams, NSRDS-NBS 46 (1973).

(4) M. Anbar, Farhataziz and A.B. Ross, NSRDS-NBS 51 (1975).

(5) Farhataziz and A.B. Ross, NSRDS-NBS 59 (1977).

(6) A.B. Ross and P. Neta, NSRDS-NBS 65 (1979).

(7) K. Sehested, J. Holcman, E. Bjergbakke and E.J. Hart, J. Phys. Chem. 88 269 (1984).

(8) H. Christensen, K. Sehested and H. Corfitzen, J. Phys. Chem. 86 1588 (1982).

(9) K. Sehested, J. Holcman, E. Bjergbakke and E.J. Hart, subm. publ. J. Phys. Chem.

(10) K. Sehested, J. Holcman and G.J. Hart, J. Phys. Chem. 87 1951 (1983).

(11) K. Sehested, J. Holcman, E. Bjergbakke and E.J. Hart, J. Phys. Chem. 86 2066 (1982).

(12) B. Hickel and K. Sehested, Private communication.

(13) G. Czapski and B.H.J. Bielski, J. Phys. Chem. 67 2180 (1963).

(14) B.L. Gall and L.M. Dorfman, J. Am. Chem. Soc. 91 2199 (1969).

(15) L. Forni, D. Bahneman and E.J. Hart, J. Phys. Chem. 86 255 (1982).

(16) J. Holcman, K. Sehested, E. Bjergbakke and E.J. Hart, J. Phys. Chem. 86 2069 (1982).

(17) J.P. Keene, Radiat. Res. 22 14 (1964).

(18) K. Sehested, E. Bjergbakke, O.L. Rasmussen and H. Fricke, J. Chem. Phys. 51 3159 (1969).

(19) W.G. Barb, J.H. Baxendale, P. George and K.R. Hargrave, Trans. Faraday Soc. 47 462 (1951).

(20) S. Navaratnam, B.J. Parsons, A.J. Swallow, Radiat. Phys. Chem. 15 159 (1980).

(21) E. Bjergbakke, S. Navaratnam, B.J. Parsons and A.J. Swallow, J. Am. Chem. Soc. 103 5926 (1981).

(22) C.A. Long and B.H.J. Bielski, J. Phys. Chem. 84 555 (1980).

(23) K. Hasegawa and P. Neta, J. Phys. Chem. 82 854 (1978).

(24) A.K. Held, D.J. Halko and J.K. Hurst, J. Am. Chem. Soc.100 5732 (1978).

(25) R.E. Connick, J. Am. Chem. Soc. 69 1509 (1947).

(26) G.G. Jayson, B.J. Parsons and A.J. Swallow, J. Chem. Soc. Faraday Trans. I 69 1597 (1973).

(27) E. Bjergbakke, Radiolysis of salt-brine (1980).

(28) M. Eigen and K. Kustin, J. Am. Chem. Soc. 84 1355 (1962).

(29) B.J. Parsons, unpublished results.

(30) T.J. Conocchioli, E.J. Hamilton and N. Sutin, J. Am. Chem. Soc. 87 926 (1965).

(31) A.T. Thornton and G.S. Laurence, J. Chem. Soc. Dalton, 804 (1973).

(32) J. Staehelin and J. Hoigné, 5th Ozon-Weltkongress, Wasser, Berlin, Collogium Verlag: West Berlin 1981.

(33) G.H. Jenks, ORNL-3848 (1965).

(34) G.H. Jenks, ORNL-4173 (1967).

(35) H. Christensen and K. Sehested, J. Phys. Chem. 87 118 (1983).

(36) K. Sehested, E. Bjergbakke and H. Fricke, Radiat. Res. 56 385 (1973).

(37) P. Cohen, Water coolant technology of power reactors. Gordon and Breach, New York 1969.

(38) N. Bibler, J. Phys. Chem. 78 211 (1974).

(39) A.O. Allen, The radiation chemistry of water and aqueous solutions. D. van Nostrand, Princeton 1961.

(40) W.G. Burns and H.E. Sims, J. Chem. Soc. Faraday Trans. I 77 2803 (1981).

(41) H. Christensen and E. Bjergbakke, STUDSVIK/NW-82/364 (1982).

Risø National Laboratory

Risø - M - 2430

Risø - M - 2430

Title and author(s)

INPUT FILES FOR COMPUTER SIMULATION OF WATER RADIOLYSIS

E. Bjergbakke, K. Sehested, O. Lang Rasmussen[x)] and H. Christensen[xx)]

[x)]Computer Installation

[xx)]Studsvik Energiteknik AB, Sweden

Date April 1984

Department or group

ACCELERATOR

Group's own registration number(s)

pages + tables + illustrations

Abstract

This report contains radiation chemistry input files for CHEMSIMUL, a program package for numerical simulation of chemical reaction systems.

Copies to

Available on request from Risø Library, Risø National Laboratory (Risø Bibliotek), Forsøgsanlæg Risø), DK-4000 Roskilde, Denmark
Telephone: (03) 37 12 12, ext. 2262. Telex: 43116

Available on request from.
Risø Library,
Risø National Laboratory, P.O. Box 49,
DK-4000 Roskilde, Denmark
Phone (02) 371212 ext. 2262

ISBN 87-550-1001-6
ISSN 0418-6435